An Explicit Third-Order Numerical Method For Size-Structured Population Equations

Tanya Kostova
Lawrence Livermore National Laboratory, L-550, 7000 East Ave., Livermore, California 94550

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A numerical method incorporating a combination of a difference scheme and several uniform and nonuniform quadrature rules is presented. The method is designed to solve size-structured population equations with linear growth rate and nonlinear fertility and mortality rates. A detailed analysis of the global discretization error is carried out. Examples with known exact solutions have been solved numerically using the proposed method. The computations show that the global error is of third order as predicted by the theory.

Keywords: structured population dynamics; error analysis; quadratures; difference schemes

1. INTRODUCTION

In this article we describe a new explicit numerical method of third order for solving size-structured equations of the form

$$\frac{\partial u}{\partial t} + \frac{\partial (g(x)u)}{\partial x} = -\mu(x, t, P(t))u(x, t), \qquad t > 0, x > 0,$$

$$g(0)u(0, t) = \int_0^X \beta(x, t, P(t))u(x, t)dx$$

$$u(x, 0) = u_0(x), \tag{1.1}$$

where

Correspondence to: Tanya Kostova, Lawrence Livermore National Laboratory, L-550, 7000 East Avenue, Livermore, CA 94550 (e-mail: kostova@llnl.gov)

$$P(t) = \int_0^X u(x, t)dx.$$

Problem (1.1) is typical for structured population dynamics, where $u(x, t)$ is a density function representing the population distribution with regard to the structuring variable x. μ and β are the mortality rate and birth function, respectively. If $g \equiv 1$, this is the so called *age-structured problem,* [1, 2].

The structuring variable x is formally named "size," but in reality it can have the physical meaning of age, size, mass, maturity level, etc.

The method is designed to find a numerical solution to (1.1) in a rectangle $\mathcal{S} = [0, X_1] \times [0, T]$, where $X_1 \geq X$. It is presumed that $\beta(x, t, P) \geq 0$, $\mu(x, t, P) \geq 0$, and that $(\partial\beta/\partial P)$ and $(\partial\mu/\partial P)$ are continuous and bounded on $\mathcal{S} \times [0, \infty)$. $g(x)$ is assumed to be continuous and such that

$$g(x) \neq 0, \qquad x \in [0, X_1], \tag{1.2}$$

and

$$g'(x) + \mu(x, t, P) \geq 0 \qquad \text{on } \mathcal{S} \times [0, \infty). \tag{1.3}$$

Additionally, for the method to have the desired $O(h^3)$ global discretization error it is necessary that the solution u and the functions β, μ have bounded derivatives up to the fourth order on a bounded set (see Theorem 3.1, Section 3.5) as well as that the growth rate g must have continuous derivatives up to the fifth order.

An abundance of articles on numerical schemes for structured equations exists in the literature, but they are designed mainly for age-dependent models. One of the first proposed methods is the popular among life scientists "escalator boxcar train method" [3]. However, its convergence and theoretical estimate of the global error has not been treated. There are quite a few other articles presenting schemes for age and size-structured equations and systems without actually proving the convergence. Though well aware of these, we further discuss only the articles with proven global error estimate, as these are the ones that would rightfully compare to the present article.

The existing numerical methods in the literature can be classified with respect to the order of the global error and to the type of equations they apply to. In [4, 5] are proposed numerical methods for the linear age-structured equation, i.e., with $\mu = \mu(a)$, $\beta = \beta(a)$. The nonlinear age-structured model (with $\mu = \mu(a, P)$, $\beta = \beta(a, P)$) was treated in several articles as follows. Methods with global approximation error $O(h)$ were published in [6–11] around the beginning of the 90s. The finite difference methods proposed in [12, 13], are of second order. Explicit second-order methods for the full nonlinear age-structured population model were proposed in [14]. These methods are based on a discretization of formula (2.2) (with $g \equiv 1$), combined with using a nonuniform open quadrature rule. This approach is related to some of the ideas used in the present article.

An explicit method of second order was also presented in [15]. However, it works for β not depending on P and also has a serious flaw: the numerical solutions can become negative, especially in problems where the solution is close to zero.

A significantly more accurate method was proposed by Milner and Rabbiolo [16]. Theirs is a method of fourth order for the linear case and of second order for the nonlinear case. The idea

is based on the observation that the linear equation can be treated as an ODE along the characteristic curves, and this idea was implemented using a Runge-Kutta procedure.

A generalization of this article followed soon in the work by Abia and Lopez-Marcos [17] in which implicit schemes utilizing Runge-Kutta modifications are formulated for the nonlinear case. The schemes are shown to have high order of convergence, but their application is expensive because of the implicitness.

Numerical methods for the linear size-structured equations were proposed in [18] (a second-order method) and [19] (of order determined by the order of the employed Runge-Kutta scheme). Numerical methods for the nonlinear case were considered in [20]. This method is proved to work for equations with nonlinear growth g and to the author's best knowledge, is unique in this respect.

To the author's best knowledge, no explicit (and therefore cheap) method of order higher than two exists for equations (1.1). It is the purpose of this article to present such a method. Our method is based on the idea of combining the already widely explored solution on the characteristics, on which all the above mentioned methods are based, with a discretization of an equation for $P(t)$, obtained by integrating (1.1). Using this equation, we calculate an approximation for $P(t)$ *first* and after that we find approximations to the solution $u(x, t)$. Calculating $P(t)$ again by using the approximate values of u will, in general, improve the accuracy of the approximation. The global discretization error of the method proposed in this article is of third order.

The article is organized as follows. Section 2 is devoted to some preliminary theoretical issues, such as derivation of the integral equation for P, summary of the quadratures used in the method, etc. Section 3 is a presentation of the method itself, consisting of the generation and approximation of the grid, the discretization formulae and their order of local approximation, and a detailed analysis of the global error. The final part of Section 3 is devoted to the construction of $O(h^3)$ approximations to the solution in the initial time layers. Section 4 contains results from a computer implementation of the method.

2. SOLVING ALONG CHARACTERISTICS

The equation

$$\frac{dx}{dt} = g(x),$$
$$x(t_0) = x_0 \tag{2.1}$$

defines the *characteristic curve* starting at the point (x_0, t_0). Let $\chi(t; x_0, t_0)$, $x_0 \geq 0$, $t_0 \geq 0$, $t \geq 0$ denote the solution of (2.1). On the characteristic curves problem (1.1) has the form

$$\frac{d}{dt}\left(u(\chi(t; x_0, t_0), t)\right) = -m(\chi(t; x_0, t_0), t, P(t))u(\chi(t; x_0, t_0), t),$$

where $m(x, t, P) = g'(x) + \mu(x, t, P)$.

Solving the above equation, we see that if (x_i, t_j) and (x_p, t_q) lie on the same characteristic curve, i.e., $x_i = \chi(t_j; x_p, t_q)$, then

$$u(x_i, t_j) = u(x_p, t_q)e^{-\int_{t_q}^{t_j} m(\chi(\tau;x_p,t_q),\tau,P(\tau))d\tau}. \tag{2.2}$$

2.1. The Equation for $P(t)$

Let us integrate (1.1) from 0 to X. We obtain the following equation for P,

$$\frac{dP}{dt} = -g(X)u(X, t) + \int_0^X [\beta(x, t, P) - \mu(x, t, P)]u(x, t)dx \tag{2.3}$$

with initial value

$$P(0) = \int_0^X u_0(x)dx.$$

Let us integrate (2.3) from t_α to t_ω for some given t_α and t_ω. We get

$$P(t_\omega) = P(t_\alpha) - g(X) \int_{t_\alpha}^{t_\omega} u(X, \tau)d\tau + \int_{t_\alpha}^{t_\omega} \int_0^X [\beta(x, \tau, P(\tau)) - \mu(x, \tau, P(\tau))]u(x, \tau)dxd\tau. \tag{2.4}$$

Denote

$$I(t) = -g(X)u(X, t) + \int_0^X [\beta(s, t, P(t)) - \mu(s, t, P(t))]u(s, t)ds. \tag{2.5}$$

Then (2.4) can be written as

$$P(t_\omega) = P(t_\alpha) + \int_{t_\alpha}^{t_\omega} I(\tau)d\tau. \tag{2.6}$$

3. QUADRATURE RULES

Because of the presence of P, obviously each numerical method for this special type of equations should incorporate quadrature rules.

In what follows, h denotes the discretization step.

3.1. Uniform Rules

We use several Newton-Cotes quadrature rules of closed and open type, of different order of discretization, namely:

A. Trapezoidal rule,

$$Trap[f] = \frac{h}{2}[f(x_0) + f(x_1)] = \int_{x_0}^{x_1} f(x)dx + \frac{1}{12}f^{(2)}(\xi)h^3; \tag{3.1}$$

B. Open formula of the rectangles,

$$R_{open}[f] = \frac{3}{2}h[f(x_1) + f(x_2)] = \int_{x_0}^{x_2} f(x)dx - \frac{3}{4}f^{(2)}(\xi)h^3; \tag{3.2}$$

C. Simpson's rule (closed formula),

$$Simp[f] = \frac{2h}{6}[f(x_0) + 4f(x_1) + f(x_2)] = \int_{x_0}^{x_2} f(x)dx + \frac{1}{90}f^{(4)}(\xi)h^5; \tag{3.3}$$

D. A 4-point closed formula,

$$F_{3/8}[f] = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] = \int_{x_0}^{x_3} f(x)dx + \frac{3}{80}f^{(4)}(\xi)h^5; \tag{3.4}$$

E. A 5-point open formula,

$$F_{4/3}[f] = \frac{4h}{3}[2f(x_1) - f(x_2) + 2f(x_3)] = \int_{x_0}^{x_4} f(x)dx - \frac{28}{90}f^{(4)}(\xi)h^5. \tag{3.4}$$

In all formulae above ξ is a value located in the integration interval. A glance at the form of the error in each formula shows that the function f must be sufficiently smooth for the quadrature rules to supply the necessary accuracy.

Composite Newton-Cotes quadrature rules are formed by splitting the interval of integration into, say, K subintervals of equal length h and using on each interval a simple quadrature formula. The discretization order of composite quadrature rules is equal to the one of the participating quadratures minus 1.

3.2. Nonuniform Rules

The nodes on the characteristic curves are not uniformly spaced (see next section), so nonuniform quadrature rules are necessary.

Let $x_0, \ldots, x_n$ be integration nodes such that $g_0 h \le |x_{i+1} - x_i| \le g_1 h$, where g_0, g_1 are constants independent of h, i. A nonuniform quadrature rule has the form

$$\int_{x_0}^{x_n} f(x)dx = \sum_{i=0}^{n} \hat{q}_i f(x_i) + R_n \tag{3.6}$$

where

$$|R_n| \le \frac{\max_{x\in[x_0,x_n]}|f^{n+1}(x)|}{(n+1)!}(x_n - x_0)^{n+2} = O(h^{n+2}),$$

$$\hat{q}_i = \int_{x_0}^{x_n} \frac{\omega_n(x)}{(x - x_i)\omega_n'(x_i)}\,dx,$$

and $\omega_n(x) = (x - x_0) \cdots (x - x_n)$.

Nonuniform rules are open if one or both of the end-point nodes do not participate.

Composite nonuniform quadrature formulae of order $s + 1$ on the interval $[a, b]$ are constructed by applying quadratures of order $s + 2$ on each of the subintervals making up $[a, b]$. Namely, if x_{ls+j}, $l = 0, \ldots, M - 1$, $j = 0, \ldots, s - 1$ are the integration nodes, such that $g_0 h \le |x_{i+1} - x_i| \le g_1 h$, then, applying simple nonuniform quadratures with accuracy of the order $O(h^{s+2})$ and with coefficients $\hat{q}_i^l$ on each interval $[x_{ls}, x_{(l+1)s}]$, the total error of the composite rule comes out to be of the order $O(h^{s+1})$. In such a case, the coefficients of the composite formula can be written as

$$q_{ls+j} = \begin{cases} \hat{q}_j^l, & \text{if } j = 0, \ldots, s-1, \text{ and } l = 0, \ldots, M-1, \\ \hat{q}_s^l + \hat{q}_0^{l+1}, & j = s \text{ and } l \ne M-1. \end{cases} \tag{3.7}$$

Finally, $q_{Ms} = \hat{q}_s^M$.

It is easy to establish that

$$q_i \le Ch,$$

where C is a constant independent of h, j. We shall use this estimate in the analysis of the discretization error. For example, C can be estimated as

$$C = \frac{2(g_1 s)^s}{g_0^s (s-1)!}\, g_1.$$

Our method uses values of s not bigger than 4.

3.3. The Numerical Method

3.3.1. Calculating the Grid

Let

$$\mathcal{S} = [0, X_1] \times [0, T], \qquad X_1 \ge X.$$

We shall calculate a numerical approximation to the solution of (1.1) at certain points of $\mathcal{S}$. We define these points as the grid $\hat{\mathcal{X}}$,

$$\hat{\mathcal{X}} = \{(x_i, t_j),\ i = 0, \ldots, L, \qquad j = 0, \ldots, N\},$$

where x_i and t_j are defined as follows.

Consider a characteristic curve starting at $x_0 = X$, $t_0 = 0$. Since $g(x) \ne 0$ and is continuous on $[0, X_1]$, we can carry out the following procedure. We solve (2.1) for $t < 0$, and find $T_l < 0$ such that $\chi(T_l; X, 0) = 0$. Let $|T_l|/K = h$, where $K = 3M + 4$, M is an integer, and h is the discretization step. Now, let $x_i = \chi(T_l + ih; 0, T_l)$, $i = 0, \ldots, K$. Obviously, $x_0 = 0$, $x_K = X$. Further, let L be such that $x_L = \chi(T_l + Lh; 0, T_l) < X_1 < x_{L+1} = \chi(T_l + (L+1)h; 0, T_l)$. Further, let N be such that $Nh < T < (N+1)h$. We shall find numerical approximations to $u(x_i, t_j)$, $i = 0, \ldots, L$, $j = 0, \ldots, N$.

It is easy to see that each pair (x_i, t_j) and (x_{i+1}, t_{j+1}), $i = 0, \ldots, L-1, j = 0, \ldots, N-1$ is located on the same characteristic curve. The grid is rectangular (i.e., the grid points are vertices of rectangles), but is not uniform (i.e., the rectangles are not equal). Because $g(x)$ is continuous and positive on $[0, X]$ and since

$$h = \int_{x_i}^{x_{i+1}} \frac{1}{g(x)}\, dx,$$

it follows that

$$h \min_{x\in[0,X]} g(x) = hg_0 \le |x_{i+1} - x_i| \le hg_1 = h \max_{x\in[0,X]} g(x). \tag{3.8}$$

Recall that the above estimate is necessary to hold in order to apply nonuniform quadrature rules (see the previous section).

3.3.2. Approximating the Grid

The grid $\hat{\mathcal{F}}$, as defined in the previous section, must be approximated itself. In our case this can be done *before* the calculation of the solution of (1.1). We find numerically a set of points (y_i, t_j), $i = 0, \ldots, L, j = 0, \ldots, N$, approximating the grid nodes (x_i, t_j) by solving equation (2.1) and using a suitable discretization method. In what follows further we assume that $y_i = x_i + O(h^4)$, whereas t_j are assumed to be exactly known.

Following this procedure, we obtain the *approximate grid*

$$\hat{\mathcal{F}} = \{(y_i, t_j),\ i = 0, \ldots, L,\ j = 0, \ldots, N\}.$$

3.3.3. The Method

The method is based on successive discretizations of formulae (2.6) and (2.2).

Equation (2.6) is discretized by using quadrature formulae with step h. The time integrals are discretized using a 5-point open Newton-Cotes rule (3.5), thus obtaining explicit formulae. The integrals in s (2.5) are discretized using a nonuniform composite rule with accuracy $O(h^4)$. The composite rule is constructed as follows. Since the number of points is $K + 1 = 3M + 5$, an open nonuniform rule involving only y_1, y_2, y_3, y_4 is used for the first 5 points y_0, y_1, y_2, y_3, y_4 and further, closed 4-point rules are used for each of the set of points $y_{4+3s}, y_{5+3s}, y_{6+3s}, y_{4+3(s+1)}$, $s = 0, \ldots, M-1$. Each of the 4-point rules have accuracy $O(h^5)$. The open 5-point rule is of accuracy $O(h^5)$, thus the composite rule is of order $O(h^4)$.

More specifically, assume that the solution $u(x, t)$ is continuous and denote

$$P_{\max} = X \max_{(x,t)\in\mathcal{S}} u(x, t).$$

Obviously, $P_{\max}$ is an upper estimate for $P(t)$.

If

$$\frac{\partial^4 u}{\partial t^4} \in C(\mathcal{S}), \qquad \frac{\partial^4 \beta}{\partial P^4}, \frac{\partial^4 \mu}{\partial P^4} \in C(\mathcal{S} \times [0, P_{\max}]), \tag{3.9}$$

and if $t_s = sh$, $s = 0, \ldots, N$ and $I_s = I(t_s)$, then

$$P(t_j) = P(t_{j-4}) + \tfrac{4}{3} h(2I_{j-3} - I_{j-2} + 2I_{j-1}) + E_1^j, \tag{3.10}$$

where $|E_1^j| \le C_1 h^5$ and C_1 is constant, depending on $\max_{t\in[0,T]}|[\partial^4 I(t)/\partial t^4]|$, but independent of h, j.

If

$$\frac{\partial^4 u}{\partial x^4} \in C(\mathcal{S}), \qquad \frac{\partial^4 \beta}{\partial x^4}, \frac{\partial^4 \mu}{\partial x^4} \in C(\mathcal{S} \times [0, P_{\max}]), \tag{3.11}$$

then $I(t_s)$ are approximated as follows (recall that $x_K = X$),

$$I_s = -g(x_K)u(x_K, t_s) + \sum_{l=1}^{K} q_l[\beta(x_l, t_s, P(t_s)) - \mu(x_l, t_s, P(t_s))]u(x_l, t_s) + E_2^s, \; s = 0, \ldots, N, \tag{3.12}$$

where $|E_2^s| \le C_2 h^4$ and C_2 is a constant depending on

$$\max_{(x,t)\in\mathcal{S}} \left| \frac{\partial^4}{\partial x^4} \{[\beta(x, t, P(t)) - \mu(x, t, P(t))]u(x, t)\} \right|.$$

The coefficients q_l are calculated as follows. Denote

$$\Phi_s(x; x_i) = \frac{\omega_s(x)}{(x - x_i)\omega_s'(x_i)}$$

and

$$\omega_s(x) = (x - x_{3s+1}) \cdots (x - x_{3s+4}), \qquad s = 0, 1, \ldots, M.$$

Then

$$q_0 = 0,$$

$$q_r = \int_0^{x_4} \Phi_0(x; x_r)dx, \qquad r = 1, 2, 3,$$

$$q_4 = \int_0^{x_4} \Phi_0(x; x_4)dx + \int_{x_4}^{x_7} \Phi_1(x; x_4)dx,$$

$$q_{3s+1} = \int_{x_{3s-2}}^{x_{3s+1}} \Phi_{s-1}(x;\, x_{3s+1})dx + \int_{x_{3s-1}}^{x_{3s+4}} \Phi_s(x;\, x_{3s+1})dx, \qquad s = 2, \ldots, M,$$

$$q_{3s+r} = \int_{x_{3s+1}}^{x_{3s+4}} \Phi_s(x;\, x_{3s+r})dx, \qquad s = 1, \ldots, M;\ r = 2, 3, 4. \tag{3.13}$$

The sum in (3.12) represents the nonuniform rule.

Further, we approximate $u(x_i, t_j)$. Assuming also that

$$\frac{d^5 g}{dx^5} \in C([0, X_1]), \tag{3.14}$$

we use the following discretization of (2.2):

$$u(x_i, t_j) = u(x_{i-2}, t_{j-2})e^{-(h/3)[m(x_{i-2},t_{j-2},P(t_{j-2}))+4m(x_{i-1},t_{j-1},P(t_{j-1}))+m(x_i,t_j,P(t_j))]} + O(h^5),\ L \geq i \geq 2,\ i \neq 3,\ N \geq j \geq 2$$

$$u(x_3, t_j) = u(0, t_{j-3})e^{-(3/8)h[m(x_0,t_{j-3},P_{j-3})+3m(x_1,t_{j-2},P_{j-2})+3m(x_2,t_{j-1},P_{j-1})+m(x_3,t_j,P_j)]} + O(h^5),$$

$$u(x_1, t_j) = u(0, t_{j-1})e^{-(h/2)[m(x_0,t_{j-1},P(t_{j-1}))+m(x_1,t_j,P(t_j))]} + O(h^3),$$

$$g(0)u(0, t_j) = \sum_{l=1}^{K} q_l \beta(x_l, t_j, P(t_j))u(x_l, t_j) + O(h^4). \tag{3.15}$$

The estimates of the discretization order rely on the assumption that the values at the preceding points (i.e., $P(t_{j-n})$, $u(x_{i-n}, t_{j-n})$) are known exactly. The expressions $O(h^q)$ above are used to denote the approximation errors, which are of the form $|E_i^j| \leq C_p h^q$ and C_p are constants independent of i, j, and h but dependent on $\max_{(x,t)\in\mathcal{S}\times[0,P_{\max}]}\left|(\partial^4/\partial x^4)u(x,\ t,\ P(t))\right|$, $\max_{(x,t)\in\mathcal{S}\times[0,P_{\max}]}\left|(\partial^i/\partial t^i)m(x, t, P(t))\right|$, $i = 2, 4$, $\max_{(x,t)\in\mathcal{S}\times[0,P_{\max}]}\left|(\partial^i/\partial x^i)\{\beta(x, t, P(t))u(x, t)\}\right|$, $i = 2, 4$.

3.4. The Numerical Scheme

First we continue β and μ for negative values of P as

$$\beta(x, t, P) = \beta(x, t, -P), \qquad \mu(x, t, P) = \mu(x, t, -P).$$

Obviously, β and μ are bounded and nonnegative, $m = \mu + g'$ is nonnegative and $(\partial\beta/\partial P)$ and $(\partial\mu/\partial P)$ are continuous and bounded on $\mathcal{S} \times [0, \infty]$ with the exception of the line $P = 0$, where $(\partial\beta/\partial P)$ and $(\partial\mu/\partial P)$ may be discontinuous.

We introduce the grid functions $\tilde{u}_i^j$, $i = 0, \ldots, L$; $j = 0, \ldots, N$, defined on $\tilde{\mathcal{X}}$ and $\tilde{P}_j$, defined on $I = \{0, \ldots, t_N\}$. For $j \geq 4$ we use the following scheme to find the values of the grid functions, using the uniform and the nonuniform quadrature rules.

$$\tilde{P}_j = \tilde{P}_{j-4} + \tfrac{4}{3}h(2\tilde{I}_{j-3} - \tilde{I}_{j-2} + 2\tilde{I}_{j-1}), \tag{3.16}$$

where

$$\tilde{I}_s = -g(X)\tilde{u}_K^s + \sum_{l=1}^{K} \tilde{q}_l[\beta(y_l, s, \tilde{P}_s) - \mu(y_l, s, \tilde{P}_s)]\tilde{u}_l^s, \tag{3.17}$$

and $\tilde{q}_l$ are defined by using formulae (3.13) with y_i instead of x_i.

$$\tilde{u}_i^j = \tilde{u}_{i-2}^{j-2} e^{-(h/3)[m(y_{i-2},t_{j-2},\tilde{P}_{j-2})+4m(y_{i-1},t_{j-1},\tilde{P}_{j-1})+m(y_i,t_j,\tilde{P}_j)]}, \qquad i \neq 0, 1, 3,\ i \leq L,\ 4 \leq j \leq N;$$

$$\tilde{u}_3^j = \tilde{u}_0^{j-3} e^{-(3/8)h[m(y_0,t_{j-3},\tilde{P}_{j-3})+3m(y_1,t_{j-2},\tilde{P}_{j-2})+3m(y_2,t_{j-1},\tilde{P}_{j-1})+m(y_3,t_j,\tilde{P}_j)]},$$

$$\tilde{u}_1^j = \tilde{u}_0^{j-1} e^{-(h/2)[m(y_0,t_{j-1},\tilde{P}_{j-1})+m(y_1,t_j,\tilde{P}_j)]},$$

$$\tilde{u}_0^j = \frac{1}{g(0)} \sum_{l=1}^{K} \tilde{q}_l \beta(y_l, t_j, \tilde{P}_j)\tilde{u}_l^j. \tag{3.18}$$

For $j = 0, 1, 2, 3$ we use initial values defined later through the *initialization process* (see Section 3.6).

3.5. An Estimate for the Global Discretization Error

In this section we show that the global discretization error of the numerical scheme depends on the accuracy of the initial values but is not better than $O(h^3)$. Let us denote

$$\eta_j = \tilde{P}_j - P(t_j);$$

$$\varepsilon_i^j = \tilde{u}_i^j - u(x_i, t_j);$$

$$\zeta_j = \tilde{I}_j - I_j;$$

$$\sigma_j = h \sum_{l=1}^{K} |\varepsilon_l^j|,$$

$$i = 0, \ldots, L,\ j = 0, \ldots, N. \tag{3.19}$$

Theorem 3.1. *Consider the discretization scheme* (3.16–3.18) *with* β *and* μ *defined as in section* 3.4. *Let* β, μ, $(\partial\beta/\partial P)$, *and* $(\partial\mu/\partial P)$ *be continuous and bounded on* $\mathcal{S} \times [0, \infty)$. *Suppose that the assumptions* (1.2), (1.3), (3.9), (3.11), *and* (3.14) *hold. Then for* $j \geq 4$ *the following discretization error estimates hold:*

$$|\eta_j| \leq W_1 h^3 + W_2\Big(\max_{i=0,1,2,3} |\eta_i| + \max_{l=0,\ldots,L}\ \max_{j=0,1,2,3} |\varepsilon_l^j|\Big), \tag{3.20}$$

$$|\varepsilon_i^j| \leq W_3 h^3 + W_4\Big(\max_{i=0,1,2,3} |\eta_i| + \max_{l=0,\ldots,L}\ \max_{j=0,1,2,3} |\varepsilon_l^j|\Big), \tag{3.21}$$

where W_s, $s = 1, 2, 3, 4$ *are constants, independent of* h, j, i.

Proof: Subtracting (3.10) from (3.16), we get

$$|\eta_j| \le |\eta_{j-4}| + \tfrac{4}{3}h|[2\zeta_{j-3} - \zeta_{j-2} + 2\zeta_{j-1}]| + C_1h^5, \qquad j \le N. \tag{3.22}$$

Subtracting (3.12) from (3.17), we get

$$|\zeta_s| \le g(X)|\varepsilon_K^s| + \sum_{l=1}^{K} |(q_l - \tilde{q}_l)|\beta_l^s u_l^s + \tilde{q}_l\tilde{\beta}_l^s|\varepsilon_l^s| + \tilde{q}_l u_l^s|\beta_l^s - \tilde{\beta}_l^s| + \sum_{l=1}^{K} |(q_l - \tilde{q}_l)|\mu_l^s u_l^s + \tilde{q}_l\tilde{\mu}_l^s|\varepsilon_l^s| + \tilde{q}_l u_l^s|\mu_l^s - \tilde{\mu}_l^s| + C_2h^4, \tag{3.23}$$

where we have denoted $f_l^s = f(x_l, t_s, P(t_s))$, $\tilde{f}_l^s = f(x_l, t_s, \tilde{P}_s)$.

Taking into consideration that β, μ, $(\partial\beta/dP)$, $(\partial\mu/dP)$ are bounded on $\mathcal{S} \times [0, \infty)$ and $u(x, t)$ is bounded on $\mathcal{S}$, and that

$$\tilde{q}_l = O(h), \quad |(q_l - \tilde{q}_l)| = O(h^5), \quad \text{and} \quad |x_l - y_l| = O(h^4), \tag{3.24}$$

we can write

$$|\zeta_s| \le g(X)|\varepsilon_K^s| + A|\eta_s| + B|\sigma_s| + C_2h^4, \tag{3.25}$$

where A, B, C_1, C_2 are positive constants, independent of h and s. In the derivation of the above estimate we have used also that $(\partial\beta/dP)$, $(\partial\mu/dP)$ are continuous with the exception of the line $P = 0$. It is easy to see that the possible discontinuity is not an obstacle to the derivation of the estimate.

In what follows we assume without loss of generality that the step h is less than some maximum value, say $h_{\max}$. Each time when we use the expression "the constant C is independent of h," the meaning is "the constant C is the same for all $h \le h_{\max}$." If $C_3 = C_1h_{\max} + C_2$, then

$$|\eta_j| \le |\eta_{j-4}| + \tfrac{4}{3}h\{A[2|\eta_{j-3}| + |\eta_{j-2}| + 2|\eta_{j-1}|] + B[2|\sigma_{j-3}| + |\sigma_{j-2}| + 2|\sigma_{j-1}|] + g(X)[2|\varepsilon_K^{j-3}| + |\varepsilon_K^{j-2}| + 2|\varepsilon_K^{j-1}|]\} + C_3h^5, \tag{3.26}$$

and C_3 is independent of h and j.

Subtracting (3.15) from (3.18) and taking into consideration that $m \ge 0$ and β, $(\partial\beta/\partial P)$, and $(\partial\mu/\partial P)$ are bounded and (3.24) we get

$$\begin{aligned}
&|\varepsilon_i^j| \le |\varepsilon_{i-2}^{j-2}| + hD[|\eta_{j-2}| + |\eta_{j-1}| + |\eta_j|] + C_4h^5, \qquad i, j > 2;\\
&|\varepsilon_3^j| \le |\varepsilon_0^{j-3}| + hE[|\eta_{j-3}| + |\eta_{j-2}| + |\eta_{j-1}|] + |\eta_j|] + C_5h^5;\\
&|\varepsilon_1^j| \le |\varepsilon_0^{j-1}| + hH[|\eta_{j-1}| + |\eta_j|] + C_6h^3;\\
&|\varepsilon_0^j| \le G|\eta_j| + P|\sigma_j| + C_7h^4,
\end{aligned} \tag{3.27}$$

where C_i, D, E, H, G, P are positive constants independent of h and j.

By substituting the estimate for $|\varepsilon_0^j|$ in the first three inequalities of (3.27), we get

$$|\varepsilon_1^j| \le G|\eta_{j-1}| + P|\sigma_{j-1}| + hH[|\eta_{j-1}| + |\eta_j|] + C_8h^3;$$
$$|\varepsilon_2^j| \le G|\eta_{j-2}| + P|\sigma_{j-2}| + hD[|\eta_{j-2}| + |\eta_{j-1}|] + |\eta_j|] + C_9h^4;$$
$$|\varepsilon_3^j| \le G|\eta_{j-3}| + P|\sigma_{j-3}| + hF[|\eta_{j-3}| + |\eta_{j-2}| + |\eta_{j-1}| + |\eta_j|] + C_{10}h^4, \quad (3.28)$$

where F and C_i, $i = 8, \ldots, 10$ are positive constants independent of h, j.

From (3.27_1) we get that for $i \ge 4$, $j \ge 4$ it holds:

$$|\varepsilon_i^j| \le |\varepsilon_{i-4}^{j-4}| + 2hD[|\eta_{j-4}| + |\eta_{j-3}| + |\eta_{j-2}| + |\eta_{j-1}| + |\eta_j|] + C_{11}h^5. \quad (3.29)$$

We now consider $|\varepsilon_K^s|$ and reiterate (3.27_1) until we get for $s \ge K$

$$|\varepsilon_K^s| \le \cdots \le |\varepsilon_0^{s-K}| + 2hD\{|\eta_{s-K}| + \cdots + |\eta_s|\} + C_{11}^1h^4, \quad (3.30)$$

and for $s < K$:

$$|\varepsilon_K^s| \le \cdots \le |\varepsilon_{K-s+\alpha}^{\alpha}| + 2hD\{|\eta_\alpha| + \cdots + |\eta_s|\} + C_{11}^1h^4, \quad (3.31)$$

where α takes the value 0 or 1 and $C_{11}^1 = C_{11}Nh = C_{11}T$.

If $s \ge K$, (3.28) and (3.27) give

$$|\varepsilon_0^{s-K}| \le G|\eta_{s-K}| + P|\sigma_{s-K}| + C_7^2h^4. \quad (3.32)$$

If $s < K$, $|\varepsilon_{K-s+\alpha}^{\alpha}|$, $\alpha = 0, 1$ is of the order determined by the initialization process (see next section).

We combine (3.30) and (3.31) using (3.32) to write:

$$|\varepsilon_K^s| \le G|\eta_{s-K}| + P|\sigma_{s-K}| + 2hD_1(|\eta_s| + \cdots + |\eta_0|) + |\varepsilon_{K-s}^0| + |\varepsilon_{K-s+1}^1| + C_{11}^3h^4, \quad (3.33)$$

where $\varepsilon_\gamma^\delta = 0$, $\eta_\kappa = 0$, $\sigma_\kappa = 0$, whenever $\gamma < 0$, or $\kappa < 0$.

Therefore from (3.26) and (3.33) we get

$$\begin{aligned}|\eta_j| \le |\eta_{j-4}| + \tfrac{8}{3}h\{&A[|\eta_{j-3}| + |\eta_{j-2}| + |\eta_{j-1}|] + B[|\sigma_{j-3}| + |\sigma_{j-2}| + |\sigma_{j-1}|] \\ &+ g(X)[G(|\eta_{j-3-K}| + |\eta_{j-2-K}| + |\eta_{j-1-K}|) + P(|\sigma_{j-3-K}| + |\sigma_{j-2-K}| + |\sigma_{j-1-K}|)]\} \\ &+ g(X)\{8h(\max_{0\le n\le K}|\varepsilon_n^0| + \max_{0\le n\le K}|\varepsilon_n^1|) + 16Dh^2[|\eta_{j-1}| + \cdots + |\eta_0|]\} + C_{11}^4h^5, \quad (3.34)\end{aligned}$$

where $\eta_\kappa = 0$, $\sigma_\kappa = 0$, whenever $\kappa < 0$.

Let $j \ge 4$. Summing up (3.28) and (3.29) for $i \ge 4$, multiplying the sum by h and renaming some constants, we get

$$\begin{aligned}|\sigma_j| \le |\sigma_{j-4}| + hP[|\sigma_{j-1}| + |\sigma_{j-2}| + |\sigma_{j-3}|] + hG[|\eta_{j-3}| + |\eta_{j-2}| + |\eta_{j-1}|] \\ + h^2Q[|\eta_{j-4}| + |\eta_{j-3}| + |\eta_{j-2}| + |\eta_{j-1}| + |\eta_j|] + C_{12}h^4. \quad (3.35)\end{aligned}$$

In the last several expressions, Q, D_1, C_{11}, C_{11}^1, C_{11}^2, C_{11}^3, C_{11}^4, and C_{12} are positive constants independent of h, j.

Let us denote $\rho_j = |\sigma_j| + |\eta_j|$.

We rewrite (3.34) as

$$|\eta_j| \le |\eta_{j-4}| + hU_1(\rho_{j-3} + \rho_{j-2} + \rho_{j-1}) + hU_2(\rho_{j-3-K} + \rho_{j-2-K} + \rho_{j-1-K}) + h^2U_3(|\eta_{j-1}| + \cdots + |\eta_0|) + Rh(\max_{0\le n\le K}|\varepsilon_n^0| + \max_{0\le n\le K}|\varepsilon_n^1|) + C_{11}^4h^4. \quad (3.36)$$

where U_i and R are constants, independent of j, h.

We substitute $|\eta_j|$ in (3.35) with its upper estimate, and write

$$|\sigma_j| \le |\sigma_{j-4}| + hV_1(\rho_{j-4} + \rho_{j-3} + \rho_{j-2} + \rho_{j-1}) + h^2Q\{|\eta_{j-4}| + hU_1(\rho_{j-3} + \rho_{j-2} + \rho_{j-1}) + hU_2(\rho_{j-3-K} + \rho_{j-2-K} + \rho_{j-1-K}) + h^2U_3(|\eta_{j-1}| + \cdots + |\eta_0|) + C_{11}^3h^4\} + RQh^3(\max_{0\le n\le K}|\varepsilon_n^0| + \max_{0\le n\le K}|\varepsilon_n^1|) + C_{12}^1h^4. \quad (3.37)$$

where C_{12}^1, V_i are constants, independent of j, h.

We now add (3.36) and (3.37) to obtain after renaming some constants:

$$\rho_j \le \rho_{j-4} + hY_1[\rho_{j-1} + \rho_{j-2} + \rho_{j-3} + \rho_{j-4} + \rho_{j-1-K} + \rho_{j-2-K} + \rho_{j-3-K}] + h^2Y_2(\rho_{j-1} + \cdots + \rho_0) + hS(\max_{0\le n\le K}|\varepsilon_n^0| + \max_{0\le n\le K}|\varepsilon_n^1|) + C_{13}h^4, \quad (3.38)$$

where S is a constant independent of h and j and $\rho_\alpha = 0$, whenever $\alpha < 0$.

Reiterating the inequality and renaming some constants, we get

$$\rho_j \le \rho_{q_j} + ST(\max_{0\le n\le K}|\varepsilon_n^0| + \max_{0\le n\le K}|\varepsilon_n^1|) + hZ[\rho_{j-1} + \cdots + \rho_0] + C_{14}h^3, \quad (3.39)$$

where Z, C_{13}, C_{14}, and Y_1, Y_2 are positive constants independent of h, j, and q_j is an integer taking one of the values 0, 1, 2, or 3.

Applying a discrete Gronwall inequality, [21], p. 41, we conclude that

$$\begin{aligned}\rho_j &\le \{C_{14}h^3 + \rho_{q_j} + ST(\max_{0\le n\le K}|\varepsilon_n^0| + \max_{0\le n\le K}|\varepsilon_n^1|)\}(1 + hZ)^j \\ &< [C_{14}h^3 + \rho_{q_j} + ST(\max_{0\le n\le K}|\varepsilon_n^0| + \max_{0\le n\le K}|\varepsilon_n^1|)]\left(1 + \frac{T}{N}Z\right)^N \\ &< [C_{14}h^3 + \rho_{q_j} + ST(\max_{0\le n\le K}|\varepsilon_n^0| + \max_{0\le n\le K}|\varepsilon_n^1|)]e^{TZ}. \end{aligned} \quad (3.40)$$

Since

$$\max_{j=0,1,2,3}\rho_{q_j} \le \max_{j=0,1,2,3}|\tilde{P}_i - P(t_i)| + T_l \max_{l=0,\ldots,K}\max_{j=0,1,2,3}|\tilde{u}_l^j - u(x_l, t_j)|,$$

(as $Kh = T_l$; see Section 3.3.1), then

$$|\eta_j| \le \{C_{14}h^3 + \max_{i=0,1,2,3} |\tilde{P}_i - P(t_i)| + (T_l + ST) \max_{l=0,\ldots,K} \max_{j=0,1,2,3} |\tilde{u}_l^j - u(x_l, t_j)|\}e^{TZ},$$

$$|\sigma_j| \le \{C_{14}h^3 + \max_{i=0,1,2,3} |\tilde{P}_i - P(t_i)| + (T_l + ST) \max_{l=0,\ldots,K} \max_{j=0,1,2,3} |\tilde{u}_l^j - u(x_l, t_j)|\}e^{TZ}. \quad (3.41)$$

Let us turn back now to (3.27), denoting $T_l + ST = S_*$. For $i > 1$, $i \neq 3$, $j > 2$,

$$|\varepsilon_i^j| \le |\varepsilon_{i-2}^{j-2}| + 3hD\{C_{14}h^3 + \max_{i=0,1,2,3} |\tilde{P}_i - P(t_i)| + S_* \max_{l=0,\ldots,K} \max_{j=0,1,2,3} |\tilde{u}_l^j - u(x_l, t_j)|\}e^{TZ} + C_4h^5$$

$$\le |\varepsilon_{r_i}^{p_j}| + C_{15}h^3 + C_{16}\{\max_{j=0,1,2,3} |\tilde{P}_i - P(t_i)| + \max_{l=0,\ldots,K} \max_{j=0,1,2,3} |\tilde{u}_l^j - u(x_l, t_j)|\}, \quad (3.42)$$

where C_{15} and C_{16} are positive constants independent of h, j and either $r_i = 0$ or $p_j = 0$ or 1.

Taking into consideration the last equation in (3.27) and the first one of (3.28) together with (3.41), we conclude that

$$|\varepsilon_i^j| \le C_{17}h^3 + C_{18}\{\max_{j=0,1,2,3} |\tilde{P}_i - P(t_i)| + \max_{l=0,\ldots,L} \max_{j=0,1,2,3} |\tilde{u}_l^j - u(x_l, t_j)|\}, \quad (3.43)$$

where C_{17} and C_{18} are positive constants independent of h, j.

A similar estimate is obtained for $|\varepsilon_0^j|$ and then for $|\varepsilon_1^j|$, $|\varepsilon_3^j|$.

This concludes the proof. ∎

So, the global error of the method depends on the local error of the first 4-time layers, but cannot be of order higher than 3.

In the next section we show how we can find initial approximations for the first several time layers.

3.6. The Initialization

The initialization is a process of finding sufficiently accurate approximations for the solution in the first 4-time layers. It can be done in various ways. Here we describe the initialization used in our implementation.

We first calculate

$$\tilde{P}_0 = \sum_{l=1}^{K} \tilde{q}_l u_0(y_l). \quad (3.44)$$

Obviously,

$$\tilde{P}_0 = P(0) + O(h^4).$$

The error comes from the numerical quadrature and the inaccuracy of the nodes and the coefficients q_l.

Further, we calculate

$$\tilde{P}_1 = \tilde{P}_0 - hg(X)u_0(X) + h\sum_{l=1}^{K} \tilde{q}_l[\beta(y_l, 0, \tilde{P}_0) - \mu(y_l, 0, \tilde{P}_0)]u_0(y_l). \tag{3.45}$$

Then $\tilde{P}_1 - P(t_1) = O(h^2)$.
Further,

$$\tilde{u}_i^1 = u_0(y_{i-1})e^{-(h/2)[m(y_{i-1},0,\tilde{P}_0)+m(y_i,t_1,\tilde{P}_1)]}, \qquad i = 1, \ldots, L,$$

for which one can establish easily that

$$|\tilde{u}_i^1 - u(x_i, t_1)| = O(h^3).$$

Next we improve the accuracy of $\tilde{P}$ by the following trick. Let $\tilde{P}_1 = P_1^{old}$ and let us apply a trapezoid rule in time and an open nonuniform rule in space.

$$\tilde{P}_1 = \tilde{P}_0 + \frac{h}{2}\left\{ -g(X)[u_0(X) + \tilde{u}_K^1] + \sum_{l=1}^{K} \tilde{q}_l[\beta(y_l, 0, \tilde{P}_0) - \mu(y_l, 0, \tilde{P}_0)]u_0(y_l) + \sum_{l=1}^{K} \tilde{q}_l[\beta(y_l, t_1, \tilde{P}_1^{old}) - \mu(y_l, t_1, \tilde{P}_1^{old})]\tilde{u}_l^1 \right\}. \tag{3.46}$$

Subtracting $\tilde{P}_1$ and $P(t_1)$, one sees that the new value of $\tilde{P}_1$ is more accurate:

$$\tilde{P}_1 - P(t_1) = O(h^3).$$

We cannot improve the accuracy of $\tilde{P}^1$ any more in the above iterative way, because the third-order error comes from the trapezoid rule in the exponential when calculating $\tilde{u}_l^1$. A more accurate rule cannot be applied at this layer (first t-layer) because we do not have more than two available values of P.

We calculate finally

$$\tilde{u}_0^1 = \frac{1}{g(0)}\sum_{l=1}^{K} \tilde{q}_l\beta(y_l, t_1, \tilde{P}_1)\tilde{u}_l^1 = u(0, h) + O(h^3). \tag{3.47}$$

Now we find $\tilde{P}_2$ by using the midpoint rule in the discretization of the time integrals:

$$\tilde{P}_2 = \tilde{P}_0 + 2h\left\{ -g(X)\tilde{u}_K^1 + \sum_{l=1}^{K} \tilde{q}_l[\beta(y_l, t_1, \tilde{P}_1) - \mu(y_l, t_1, \tilde{P}_1)]\tilde{u}_l^1 \right\}, \tag{3.48}$$

which can be written as

$$\tilde{P}_2 = \tilde{P}_0 + 2h\tilde{I}_1.$$

Then one can find that

$$|\tilde{P}_2 - P(t_2)| = O(h^3).$$

Further, u_i^2 is calculated as

$$\begin{aligned} \tilde{u}_i^2 &= u_0(y_{i-2})e^{-(h/3)[m(y_{i-2},0,\tilde{P}_0)+4m(y_{i-1},t_1,\tilde{P}_1)+m(y_i,t_2,\tilde{P}_2)]}, \qquad \text{for } i \geq 2, \\ \tilde{u}_1^2 &= u_0^1 e^{-(h/2)[m(0,t_1,\tilde{P}_1)+m(y_1,t_2,\tilde{P}_2)]}. \end{aligned} \tag{3.49}$$

One can find that

$$\begin{aligned} \tilde{u}_i^2 &= u(x_i, t_2) + O(h^4), \qquad i \geq 2, \\ \tilde{u}_1^2 &= u(x_1, t_2) + O(h^3). \end{aligned} \tag{3.50}$$

Finally, we calculate u_0^2:

$$\tilde{u}_0^2 = \frac{1}{g(0)} \sum_{l=1}^{K} \tilde{q}_l \beta(y_l, t_2, \tilde{P}_2)\tilde{u}_l^2, \tag{3.51}$$

thus obtaining that

$$\tilde{u}_0^2 = u(0, t_2) + O(h^3).$$

We continue to obtain $\tilde{P}_3$ by using a 4-point open formula R_{open} to approximate the time integrals:

$$\tilde{P}_3 = \tilde{P}_0 + \frac{3h}{2}[\tilde{I}_1 + \tilde{I}_2], \tag{3.52}$$

thus obtaining

$$\tilde{P}_3 = P(t_3) + O(h^3).$$

We further calculate $\tilde{u}_i^3$, $i = 3, \ldots, L$ as

$$\tilde{u}_i^3 = u_{i-2}^1 e^{-(h/3)[m(y_{i-2},t_1,\tilde{P}_1)+4m(y_{i-1},t_2,\tilde{P}_2)+m(y_i,t_3,\tilde{P}_3)]},$$

thus obtaining local approximation of order $O(h^3)$.

$$\tilde{u}_i^3 = u(x_i, t_3) + O(h^3), \qquad i = 3, \ldots, L.$$

The values $\tilde{u}_1^3$ and $\tilde{u}_2^3$ are calculated with $O(h^3)$ accuracy:

$$\tilde{u}_1^3 = u_0^2 e^{-(h/2)[m(0,t_2,\tilde{P}_2)+m(y_1,t_3,\tilde{P}_3)]} = u(x_1, t_3) + O(h^3)$$
$$\tilde{u}_2^3 = u_1^2 e^{-(h/2)[m(y_1,t_2,\tilde{P}_2)+m(y_2,t_3,\tilde{P}_3)]} = u(x_2, t_3) + O(h^3) \tag{3.53}$$

Finally,

$$\tilde{u}_0^3 = \frac{1}{g(0)} \sum_{l=1}^{K} \tilde{q}_l \beta(y_l, t_3, \tilde{P}_3)\tilde{u}_l^3 = u(0, t_3) + O(h^3). \tag{3.54}$$

This concludes the initialization process.

3.7. The Magnitude of the Global Discretization Error

Combining the results of the initialization process and Theorem 3.1, we can formulate the following result.

Theorem 3.2. *If the assumptions of Theorem* 3.1 *hold, the global discretization error of the numerical scheme* (3.16–3.18) *combined with the initialization described in Section* 3.6 *is of the order* $O(h^3)$.

Going through the proof of Theorem 3.1 we can notice that the third-order of the global error is actually due to the third-order discretization error in the calculation of $u(h, t_j)$. If this layer could be calculated with a better accuracy and if the initialization could be more accurate, the algorithm would benefit by producing a higher order of the global error.

4. IMPLEMENTATION OF THE NUMERICAL ALGORITHM

A Fortran code implementing the proposed algorithm was written by the author. It works for problems with $X = X_1 = 1$, but can be easily modified for a larger class of problems. The calculations were done with double precision on a Sun Ultra 5 station.

The code calculates the grid by solving (2.1) by a Runge-Kutta fourth-order method.

The proposed method was tested on three nonlinear examples. Further, we present the examples and the results of the numerical experiments. For each problem, the solution was calculated with four different steps, each one roughly twice smaller than the previous. Because of the specific way the step is calculated, exact halving of the step cannot be achieved. Table I presents the maximum values of the errors $\eta_{\max} = \max_j \eta_j$ and $\varepsilon_{\max} = \max_{i,j} \varepsilon_i^j$. The numbers presented below have been rounded to the first several digits. Naturally, in all examples $P(t) = \int_0^1 u(x, t)dx$.

The results in Table I demonstrate the third order of the method. The reported results show that the order of the global error is actually somewhat larger than 3. This is not surprising as in the proof of the convergence theorem, we made many quite crude estimates from above.

TABLE I. Maximum errors of Problems 1, 2, 3 for decreasing discretization steps.

	Step h	$\eta_{\max}$	$\varepsilon_{\max}$
Problem 1			
	0.078	2.79×10^{-4}	1.85×10^{-4}
	0.0374	3.006×10^{-5}	2.403×10^{-5}
	0.0183	3.51×10^{-6}	3.063×10^{-6}
	0.0089	4.123×10^{-7}	3.73×10^{-7}
Problem 2			
	0.224	2.79×10^{-6}	1.05×10^{-5}
	0.11	2.69×10^{-7}	1.64×10^{-6}
	0.0547	3.24×10^{-8}	1.98×10^{-7}
	0.027	3.96×10^{-9}	2.2×10^{-8}
Problem 3			
	0.0484	2.22×10^{-3}	1.25×10^{-3}
	0.0234	1.02×10^{-4}	7.44×10^{-5}
	0.0103	5.89×10^{-6}	5.26×10^{-6}
	0.0055	4.47×10^{-7}	4.62×10^{-7}

See text for explanation.

Example 1. Problem with solutions vanishing with time.

$$u_t + (e^{-x}u)_x = -\left(1 + e^{-x} + \frac{e^{-x}\sin x}{2 + \cos x}\right)\frac{0.2 + (1 + 0.5\sin(1))e^{-t}}{0.2 + P}u, \qquad x \in (0, 1], t > 0,$$

$$u(0, t) = \int_0^1 \frac{3}{2 + \cos x}\frac{0.5 + (1 + 0.5\sin(1))e^{-t}}{0.5 + P}u(x, t)dx$$

$$u(x, 0) = 1 + \frac{\cos x}{2}, \tag{4.1}$$

The exact solution is $u(x, t) = e^{-t}[1 + (\cos x/2)]$.

The approximate solution was calculated for $t \in [0, 15]$. The values of M were, respectively, 6, 14, 30, and 63.

Example 2. Problem with solutions growing exponentially with time.

$$u_t + \left(\frac{0.1}{1 + x}u\right)_x = -\left(\frac{0.02}{(1 + x)^2} - 0.0125\right)\frac{1 + \ln(2)e^{0.125t})}{0.1 + P}u, \qquad x \in (0, 1], t > 0,$$

$$0.1u(0, t) = \int_0^1 0.1\,\frac{(1 + x)(0.5 + 0.1\,\ln(2)e^{0.125t})}{0.5 + P}u(x, t)dx$$

$$u(x, 0) = \frac{0.1}{1 + x}, \tag{4.2}$$

The exact solution is $u(x, t) = e^{0.125t[0.1/(1+x)]}$.

The solution was calculated for $t \in [0, 22]$. The values of M were, respectively, 21, 44, 90, and 185.

Example 3. Problem with solutions slowly changing in time.

$$u_t + \left(\frac{1}{1+x}\,u\right)_x = -\left(\frac{2}{(1+x)^2} + 0.001\right)\frac{0.3 + 2\ln(2)e^{-0.001t}}{0.3 + 2P}\,u, \qquad x \in (0, 1],\ t > 0,$$

$$u(0, t) = \int_0^1 \frac{(1+x)(1+\ln(2)e^{-0.001t})}{1+P}\,u(x, t)dx$$

$$u(x, 0) = \frac{1}{1+x}, \tag{4.3}$$

The exact solution is $u(x, t) = [e^{-0.001t}/(1+x)]$.

The solution was calculated for $t \in [0, 6]$. The values of M were, respectively, 9, 20, 44, and 90.

5. DISCUSSION

A method that uses the same formula for $\tilde{u}_3^j$ in (3.18) as the one for $\tilde{u}_i^j$, $i > 3$ would be of third order as well. The variation we use gives a slightly better local approximation for $\tilde{u}_3^j$ because it does not inherit the $O(h^3)$ error in $\tilde{u}_1^j$.

The question about the stability of the method was raised by one of the reviewers. This question always arises with explicit methods. We do not offer any treatment of the stability properties of the method in this article. This question could be addressed in a subsequent article. The included results from numerical experiments show that the method gives very good approximation with comparatively large steps.

Note that, to apply the method, we needed to continue μ and β for negative P and to assume boundedness of β, μ, $(\partial\beta/\partial P)$, $(\partial\mu/\partial P)$ for all P. The problem (1.1) by itself requires that the vital rates are defined only for $P \geq 0$. The continuation of β, μ becomes necessary in case that the solution tends to 0 and negative values of $\tilde{P}_i$ might appear, although these would be good approximations of $P(t_i)$.

A similar method that will always generate positive P_i (and therefore a continuation of β, μ will not be needed) can be proposed. It can be one that uses a different formula for the time discretization (3.10) of P. Such a formula can be

$$P(t_j) = P(t_{j-5}) + h\,\tfrac{5}{24}\,(11I_{j-4} + I_{j-3} + I_{j-2} + 11I_{j-1}),$$

based on the quadrature rule

$$\int_{x_0}^{x_5} f(x)dx = h\,\frac{5}{24}\,[11f(x_1) + f(x_2) + f(x_3) + 11f(x_4)] - \frac{95}{144}\,f^{(4)}(\zeta)h^5.$$

The error analysis will go along the same line as in Theorem 3.1. The price to be paid for using such a formula is to calculate one more initial time layer with accuracy $O(h^4)$. Such a method will not ease the requirements for boundedness of β, μ, and their P-derivatives.

Another issue needing discussion is the assumption (1.3). It is necessary for the proof of convergence. It may not be essential for the convergence itself. The assumption (1.2) is an important simplification. Angulo and Lopez-Marcos [19] allow $g(x)$ to become zero at one end of the size interval (say X_1). This complicates the numerical procedure making the characteristics to be densely located. These authors take special measures to avoid the grid to become too dense in some regions. Similar approach can be taken in the implementation of our method as well. The goal of this article is, however, to present the idea of using two different discretizations (for u and P), which allows to increase the order of convergence. Obviously, based on this idea, various modifications can be done further, such as methods for systems of structured equations and other types of equations, describing complex processes. When complexity of the model is an issue, the high order of convergence is a major advantage of the method.

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